Francesco Zerbetto

List of Publications by Year
in descending order

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400 papers	19,508 citations	16451 64 h-index	17105 122 g-index
422 all docs	422 docs citations	422 times ranked	16033 citing authors

#	Article	IF	Citations
1	Fullerenes against COVID-19: Repurposing C60 and C70 to Clog the Active Site of SARS-CoV-2 Protease. Molecules, 2022, 27, 1916.	3.8	11
2	Photothermal motion: effect of low-intensity irradiation on the thermal motion of organic nanoparticles. Nanoscale, 2022, 14, 7233-7241.	5.6	2
3	Green Fabrication of (6,5)Carbon Nanotube/Protein Transistor Endowed with Specific Recognition. Advanced Electronic Materials, 2021, 7, 2001114.	5.1	11
4	A Bioâ€Conjugated Fullerene as a Subcellularâ€Targeted and Multifaceted Phototheranostic Agent. Advanced Functional Materials, 2021, 31, 2101527.	14.9	22
5	Single-molecule mechanics of synthetic aromatic amide helices: Ultrafast and robust non-dissipative winding. CheM, 2021, 7, 1333-1346.	11.7	13
6	Incorporation of Molecular Nanoparticles Inside Proteins: The Trojan Horse Approach in Theranostics. Accounts of Materials Research, 2021, 2, 594-605.	11.7	20
7	Human Serum Albuminâ€“Oligothiophene Bioconjugate: A Phototheranostic Platform for Localized Killing of Cancer Cells by Precise Light Activation. Jacs Au, 2021, 1, 925-935.	7.9	19
8	Viscoelasticity and Noise Properties Reveal the Formation of Biomemory in Cells. Journal of Physical Chemistry B, 2021, 125, 10883-10892.	2.6	5
9	Dissecting the Supramolecular Dispersion of Fullerenes by Proteins/Peptides: Amino Acid Ranking and Driving Forces for Binding to C60. International Journal of Molecular Sciences, 2021, 22, 11567.	4.1	4
10	Complex Nanoparticle Diffusional Motion in Liquid-Cell Transmission Electron Microscopy. Journal of Physical Chemistry C, 2020, 124, 14881-14890.	3.1	18
11	Inhibition of Î±-chymotrypsin by pristine single-wall carbon nanotubes: Clogging up the active site. Journal of Colloid and Interface Science, 2020, 571, 174-184.	9.4	22
12	Electron Dynamics with Explicit-Time Density Functional Theory of the [4+2] Dielsâ€“Alder Reaction. Journal of Chemical Theory and Computation, 2020, 16, 2172-2180.	5.3	3
13	White and Colored Noises as Driving Forces of Electron Transfer: The Photolyase Repair Mechanism as a Test Case. Journal of Physical Chemistry Letters, 2019, 10, 4511-4516.	4.6	2
14	Oriented External Electric Fields Affect Rate and Stereoselectivity of Electrocyclic Reactions. Journal of Physical Chemistry C, 2019, 123, 26370-26378.	3.1	20
15	Retinoic acid/calcite micro-carriers inserted in fibrin scaffolds modulate neuronal cell differentiation. Journal of Materials Chemistry B, 2019, 7, 5808-5813.	5.8	11
16	Identification and preparation of stable water dispersions of protein - Carbon nanotube hybrids and efficient design of new functional materials. Carbon, 2019, 147, 70-82.	10.3	30
17	CNTâ€Catalyzed Oxidative Dehydrogenation of Ethylbenzene to Styrene: DFT Calculations Disclose the Pathways. ChemNanoMat, 2019, 5, 499-505.	2.8	5
18	Photocatalytic activity of exfoliated graphiteâ€“TiO₂ nanoparticle composites. Nanoscale, 2019, 11, 19301-19314.	5.6	18

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19	Controlling Sizeâ€Dispersion of Single Walled Carbon Nanotubes by Interaction with Polyoxometalates Armed with a Tryptophan Tweezer. European Journal of Inorganic Chemistry, 2019, 2019, 374-379.	2.0	6
20	Dynamic Self-Organization and Catalysis: Periodic versus Random Driving Forces. Journal of Physical Chemistry C, 2019, 123, 825-835.	3.1	3
21	Stable and Biocompatible Monodispersion of C₆₀ in Water by Peptides. Bioconjugate Chemistry, 2019, 30, 808-814.	3.6	18
22	Functionalization Pattern of Graphene Oxide Sheets Controls Entry or Produces Lipid Turmoil in Phospholipid Membranes. ACS Applied Materials & Interfaces, 2018, 10, 15487-15493.	8.0	16
23	Structural determinants in the bulk heterojunction. Physical Chemistry Chemical Physics, 2018, 20, 5708-5720.	2.8	3
24	Delivery systems for agriculture: Fe-EDDHSA/CaCO3 hybrid crystals as adjuvants for prevention of iron chlorosis. Chemical Communications, 2018, 54, 1635-1638.	4.1	6
25	Proteins as supramolecular hosts for C₆₀: a true solution of C₆₀ in water. Nanoscale, 2018, 10, 9908-9916.	5.6	33
26	Tackling the Challenges of Dynamic Experiments Using Liquid-Cell Transmission Electron Microscopy. Accounts of Chemical Research, 2018, 51, 3-11.	15.6	78
27	New insights into the composition of Indian yellow and its use in a Rajasthani wall painting. Microchemical Journal, 2018, 137, 238-249.	4.5	16
28	Interactions between Endohedral Metallofullerenes and Proteins: The Gd@C₆₀â€“Lysozyme Model. ACS Omega, 2018, 3, 13782-13789.	3.5	12
29	Interaction of Single Cells with 2D Organic Monolayers: A Scanning Electrochemical Microscopy Study. ChemElectroChem, 2018, 5, 2975-2981.	3.4	16
30	Temperature and Conductivity as Indicators of the Morphology and Activity of a Submarine Volcano: Avyssos (Nisyros) in the South Aegean Sea, Greece. Geosciences (Switzerland), 2018, 8, 193.	2.2	7
31	C60 Bioconjugation with Proteins: Towards a Palette of Carriers for All pH Ranges. Materials, 2018, 11, 691.	2.9	25
32	Graphene Materials Strengthen Aqueous Polyurethane Adhesives. ACS Omega, 2018, 3, 8829-8835.	3.5	12
33	Multifractal structure of microscopic eyeâ€“head coordination. Physica A: Statistical Mechanics and Its Applications, 2018, 512, 945-953.	2.6	3
34	Graphene Oxide Promotes Site-Selective Allylic Alkylation of Thiophenes with Alcohols. Organic Letters, 2018, 20, 3705-3709.	4.6	30
35	Impact of the green tea ingredient epigallocatechin gallate and a short pentapeptide (Ile-Ile-Ala-Glu-Lys) on the structural organization of mixed micelles and the related uptake of cholesterol. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 1956-1963.	2.4	3
36	Breathing modes of Kolumbo submarine volcano (Santorini, Greece). Scientific Reports, 2017, 7, 46515.	3.3	11

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37	Optical and theoretical investigation of Indian yellow (euxanthic acid and euxanthone). Dyes and Pigments, 2017, 144, 234-241.	3.7	6
38	Modeling Living Cells Response to Surface Tension and Chemical Patterns. ACS Applied Materials & Interfaces, 2017, 9, 19552-19561.	8.0	11
39	Engineering the Fullereneâ€protein Interface by Computational Design: The Sum is More than its Parts. Israel Journal of Chemistry, 2017, 57, 547-552.	2.3	14
40	Analysis of the vibronic structure of the trans-stilbene fluorescence and excitation spectra: the S₀ and S₁ PES along the C_eî€C_e and C_eâ€“C_{ph} torsions. Physical Chemistry Chemical Physics, 2017, 19, 25095-25104.	2.8	6
41	Directly Observing Micelle Fusion and Growth in Solution by Liquid-Cell Transmission Electron Microscopy. Journal of the American Chemical Society, 2017, 139, 17140-17151.	13.7	118
42	Aromatic Bromination of N-Phenylacetamide Inside CNTs. Are CNTs Real Nanoreactors Controlling Regioselectivity and Kinetics? A QM/MM Investigation. Journal of Physical Chemistry C, 2017, 121, 27674-27682.	3.1	17
43	Bioinspired Nanocomposites: Ordered 2D Materials Within a 3D Lattice. Advanced Functional Materials, 2016, 26, 5569-5575.	14.9	23
44	Time-dependent quantum simulation of coronene photoemission spectra. Physical Chemistry Chemical Physics, 2016, 18, 13604-13615.	2.8	4
45	Biorecognition in Organic Field Effect Transistors Biosensors: The Role of the Density of States of the Organic Semiconductor. Analytical Chemistry, 2016, 88, 12330-12338.	6.5	58
46	CNT-Confinement Effects on the Menshutkin S_N2 Reaction: The Role of Nonbonded Interactions. Journal of Chemical Theory and Computation, 2016, 12, 4082-4092.	5.3	21
47	Time Fractional Diffusion Equations and Analytical Solvable Models. Journal of Physics: Conference Series, 2016, 738, 012106.	0.4	1
48	Electric Field Promotes Pentacene Dimerization in Thin Film Transistors. Journal of Physical Chemistry C, 2016, 120, 13942-13947.	3.1	2
49	â€œActiveâ€•drops as phantom models for living cells: a mesoscopic particle-based approach. Soft Matter, 2016, 12, 3538-3544.	2.7	3
50	Stochastic analysis of movements on surfaces: The case of C60 on Au(111). Chemical Physics Letters, 2015, 633, 163-168.	2.6	12
51	Are Twoâ€Station Biased Random Walkers Always Potential Molecular Motors?. ChemPhysChem, 2015, 16, 104-107.	2.1	1
52	Conformation Diversity of a Fusedâ€Ring Pyrazine Derivative on Au(111) and Highly Ordered Pyrolytic Graphite. Chemistry - an Asian Journal, 2015, 10, 1311-1317.	3.3	7
53	Calcite Single Crystals as Hosts for Atomicâ€Scale Entrapment and Slow Release of Drugs. Advanced Healthcare Materials, 2015, 4, 1510-1516.	7.6	32
54	Modeling Nanotube Caps: The Relationship Between Fullerenes and Caps. Journal of Physical Chemistry A, 2015, 119, 12839-12844.	2.5	6

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55	Graphene Can Wreak Havoc with Cell Membranes. ACS Applied Materials & Interfaces, 2015, 7, 4406-4414.	8.0	142
56	In situ nanomechanical characterization of the early stages of swelling and degradation of a biodegradable polymer. Nanoscale, 2015, 7, 5403-5410.	5.6	16
57	Changes of the Molecular Structure in Organic Thin Film Transistors during Operation. Journal of Physical Chemistry C, 2015, 119, 15912-15918.	3.1	10
58	Blocking the Passage: C₆₀ Geometrically Clogs K⁺ Channels. ACS Nano, 2015, 9, 4827-4834.	14.6	41
59	Fast photodynamics of azobenzene probed by scanning excited-state potential energy surfaces using slow spectroscopy. Nature Communications, 2015, 6, 5860.	12.8	82
60	Crossover of two power laws in the anomalous diffusion of a two lipid membrane. Journal of Chemical Physics, 2015, 142, 215102.	3.0	28
61	Thermodynamics of Binding Between Proteins and Carbon Nanoparticles: The Case of C₆₀@Lysozyme. Journal of Physical Chemistry C, 2015, 119, 28077-28082.	3.1	40
62	Graphite Oxide and Aromatic Amines: Size Matters. Advanced Functional Materials, 2015, 25, 263-269.	14.9	44
63	Operations and Thermodynamics of an Artificial Rotary Molecular Motor in Solution. ChemPhysChem, 2014, 15, 1834-1840.	2.1	3
64	Imaging, photophysical properties and DFT calculations of manganese blue (barium) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 387 Td (mang 15297-15300.	4.1	12
65	Electrochemical Fabrication of Surface Chemical Gradients in Thiol Self-Assembled Monolayers with Tailored Work-Functions. Langmuir, 2014, 30, 11591-11598.	3.5	13
66	Atomistic molecular dynamics simulations reveal insights into adsorption, packing, and fluxes of molecules with carbon nanotubes. Journal of Materials Chemistry A, 2014, 2, 12123-12135.	10.3	41
67	Explaining Fullerene Dispersion by using Micellar Solutions. ChemPhysChem, 2014, 15, 2998-3005.	2.1	19
68	Redox active Double Wall Carbon Nanotubes show intrinsic anti-proliferative effects and modulate autophagy in cancer cells. Carbon, 2014, 78, 589-600.	10.3	9
69	C₆₀@Lysozyme: Direct Observation by Nuclear Magnetic Resonance of a 1:1 Fullerene Protein Adduct. ACS Nano, 2014, 8, 1871-1877.	14.6	70
70	Î±,Îµ-Hybrid Foldamers with 1,2,3-Triazole Rings: Order versus Disorder. Journal of Organic Chemistry, 2014, 79, 5958-5969.	3.2	14
71	Playing peekaboo with graphene oxide: a scanning electrochemical microscopy investigation. Chemical Communications, 2014, 50, 13117-13120.	4.1	30
72	Cl^(â¯) Exchange S_N2 Reaction inside Carbon Nanotubes: Câ€“HÂ·Â·Â·Ï€ and ClÂ·Â·Â·Ï€ Interactions Govern the Course of the Reaction. Journal of Physical Chemistry C, 2014, 118, 5032-5040.	3.1	29

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73	Customizing Properties of Î²-Chitin in Squid Pen (Gladius) by Chemical Treatments. Marine Drugs, 2014, 12, 5979-5992.	4.6	31
74	A Strongly Emitting Liquidâ€Crystalline Derivative of Y₃N@C₈₀: Bright and Longâ€Lived Nearâ€IR Luminescence from a Charge Transfer State. Angewandte Chemie - International Edition, 2013, 52, 12303-12307.	13.8	21
75	Morphological and mechanical characterization of composite calcite/SWCNTâ€“COOH single crystals. Nanoscale, 2013, 5, 6944.	5.6	20
76	An Experimentally Observed Trimetallofullerene Sm₃@I_h-C₈₀: Encapsulation of Three Metal Atoms in a Cage without a Nonmetallic Mediator. Journal of the American Chemical Society, 2013, 135, 4187-4190.	13.7	67
77	Rolling up a Graphene Sheet. ChemPhysChem, 2013, 14, 3447-3453.	2.1	49
78	And Yet it Moves! Microfluidics Without Channels and Troughs. Advanced Functional Materials, 2013, 23, 5543-5549.	14.9	22
79	The Devil and Holy Water: Protein and Carbon Nanotube Hybrids. Accounts of Chemical Research, 2013, 46, 2454-2463.	15.6	136
80	Reverse Engineering of Monolayers and Nanopatterns. Advanced Materials, 2013, 25, 449-455.	21.0	8
81	Common Force Field Thermodynamics of Cholesterol. Scientific World Journal, The, 2013, 2013, 1-7.	2.1	1
82	Temperatureâ€Dependent Fluorescence of Cu₅ Metal Clusters: A Molecular Thermometer. Angewandte Chemie - International Edition, 2012, 51, 9662-9665.	13.8	87
83	Role of Substrate in Directing the Self-Assembly of Multicomponent Supramolecular Networks at the Liquidâ€“Solid Interface. ACS Nano, 2012, 6, 8381-8389.	14.6	74
84	Engineering molecular chains in carbon nanotubes. Nanoscale, 2012, 4, 7540.	5.6	6
85	Local Ice Melting by an Antifreeze Protein. Biomacromolecules, 2012, 13, 2046-2052.	5.4	18
86	GPUâ€accelerated computation of electron transfer. Journal of Computational Chemistry, 2012, 33, 2351-2356.	3.3	7
87	Amyloid-Î² fibril disruption by C60â€”molecular guidance for rational drug design. Physical Chemistry Chemical Physics, 2012, 14, 8599.	2.8	56
88	Excitation Energy Transfer and Low-Efficiency Photolytic Splitting of Water Ice by Vacuum UV Light. Journal of Physical Chemistry Letters, 2012, 3, 3610-3615.	4.6	11
89	Structural features of aquaporin 4 supporting the formation of arrays and junctions in biomembranes. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 2234-2243.	2.6	7
90	Thermal collapse of snowflake fractals. Chemical Physics Letters, 2012, 543, 82-85.	2.6	1

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91	Shape Governs the Motion of Chemically Propelled Janus Swimmers. Journal of Physical Chemistry C, 2012, 116, 592-598.	3.1	47
92	Stability, Dynamics, and Lubrication of MoS₂ Platelets and Nanotubes. Langmuir, 2012, 28, 7393-7400.	3.5	80
93	A Simple Road for the Transformation of Few-Layer Graphene into MWNTs. Journal of the American Chemical Society, 2012, 134, 13310-13315.	13.7	58
94	Selective Enhancement of Photoluminescence in Filled Singleâ€Walled Carbon Nanotubes. Advanced Functional Materials, 2012, 22, 3202-3208.	14.9	40
95	Probing the Structure of Lysozymeâ€“Carbonâ€Nanotube Hybrids with Molecular Dynamics. Chemistry - A European Journal, 2012, 18, 4308-4313.	3.3	84
96	Conformational Selection and Folding-upon-binding of Intrinsically Disordered Protein CP12 Regulate Photosynthetic Enzymes Assembly. Journal of Biological Chemistry, 2012, 287, 21372-21383.	3.4	57
97	Fullerenol entrapment in calcite microspheres. Chemical Communications, 2011, 47, 10662.	4.1	10
98	Polymorphism and isomerisation of an azobenzene derivative on gold. Chemical Communications, 2011, 47, 8662.	4.1	3
99	The effect of temperature on the internal dynamics of dansylated POPAM dendrimers. RSC Advances, 2011, 1, 1778.	3.6	9
100	Laws of thermal diffusion of individual molecules on the gold surface. Physical Chemistry Chemical Physics, 2011, 13, 13690.	2.8	5
101	In Silico Carborane Docking to Proteins and Potential Drug Targets. Journal of Chemical Information and Modeling, 2011, 51, 1882-1896.	5.4	43
102	Fullerene sorting proteins. Nanoscale, 2011, 3, 2873.	5.6	41
103	A computational analysis of the insertion of carbon nanotubes into cellular membranes. Biomaterials, 2011, 32, 7079-7085.	11.4	53
104	Dynamics of a lipid bilayer induced by electric fields. Physical Chemistry Chemical Physics, 2011, 13, 9216.	2.8	8
105	A molecular dynamics investigation of structure and dynamics of SDS and SDBS micelles. Soft Matter, 2011, 7, 9148.	2.7	99
106	Fast Calculation of Electrostatic Potentials on the GPU or the ASIC MD-GRAPE-3. Computer Journal, 2011, 54, 1181-1187.	2.4	10
107	A RNA-based nanodevice recording temperature over time. Chemical Physics, 2010, 369, 91-95.	1.9	3
108	Dualâ€Gate Organic Fieldâ€Effect Transistors as Potentiometric Sensors in Aqueous Solution. Advanced Functional Materials, 2010, 20, 898-905.	14.9	136

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109	Controlled Hydrogenâ€Bond Breaking in a Rotaxane by Discrete Solvation. Angewandte Chemie - International Edition, 2010, 49, 3896-3900.	13.8	32
110	Electronic structure and radial breathing mode for carbon nanotubes with ultraâ€high curvature. Physica Status Solidi (B): Basic Research, 2010, 247, 2774-2778.	1.5	5
111	Nanopatterning of carbonaceous structures by field-induced carbon dioxide splitting with a force microscope. Applied Physics Letters, 2010, 96, .	3.3	43
112	Baiting Proteins with C₆₀. ACS Nano, 2010, 4, 2283-2299.	14.6	104
113	Electric Field Effects on Short Fibrils of AÎ² Amyloid Peptides. Journal of Chemical Theory and Computation, 2010, 6, 3516-3526.	5.3	39
114	Quantum Study of Laser-Induced Initial Activation of Graphite-to-Diamond Conversion. Journal of the American Chemical Society, 2010, 132, 12166-12167.	13.7	9
115	Electronic Structure of Carbon Nanotubes with Ultrahigh Curvature. ACS Nano, 2010, 4, 4515-4522.	14.6	57
116	Splitting CO₂ with Electric Fields: A Computational Investigation. Journal of Physical Chemistry Letters, 2010, 1, 3256-3260.	4.6	34
117	Internal Dynamics and Energy Transfer in Dansylated POPAM Dendrimers and Their Eosin Complexes. Journal of Physical Chemistry B, 2010, 114, 1548-1558.	2.6	15
118	What Is Adenine Doing in Photolyase?. Journal of Physical Chemistry B, 2010, 114, 4101-4106.	2.6	38
119	Molecules on gold. Chemical Communications, 2010, 46, 667-676.	4.1	28
120	Sensing Biomolecules with Ultra-Thin Film Organic Field Effect Transistors. Biophysical Journal, 2010, 98, 658a.	0.5	1
121	Hydroxyl vacancies in single-walled aluminosilicate and aluminogermanate nanotubes. Journal of Physics Condensed Matter, 2009, 21, 195301.	1.8	20
122	Dynamics of molecular self-ordering in tetraphenyl porphyrin monolayers on metallic substrates. Nanotechnology, 2009, 20, 275602.	2.6	75
123	A Carbon Nanoâ€Onionâ€“Ferrocene Donorâ€“Acceptor System: Synthesis, Characterization and Properties. Chemistry - A European Journal, 2009, 15, 4419-4427.	3.3	58
124	Quantitative analysis of charge-carrier trapping in organic thin-film transistors from transfer characteristics. Applied Physics A: Materials Science and Processing, 2009, 95, 55-60.	2.3	17
125	FTâ€Raman characterization of the antipodal bisâ€adduct of C₆₀ and anthracene. Physica Status Solidi (B): Basic Research, 2009, 246, 2794-2797.	1.5	5
126	Wrapping Nanotubes with Micelles, Hemimicelles, and Cylindrical Micelles. Small, 2009, 5, 2191-2198.	10.0	77

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127	Introducing temperature dependence in an enhanced Poissonâ€“Boltzmann approach. Chemical Physics Letters, 2009, 480, 313-317.	2.6	7
128	Intermolecular Repulsion through Interfacial Attraction: Toward Engineering of Polymorphs. Journal of the American Chemical Society, 2009, 131, 15655-15659.	13.7	32
129	Multistate Photo-Induced Relaxation and Photoisomerization Ability of Fumaramide Threads: A Computational and Experimental Study. Journal of the American Chemical Society, 2009, 131, 104-117.	13.7	27
130	Water-induced polaron formation at the pentacene surface: Quantum mechanical molecular mechanics simulations. Physical Review B, 2009, 79, .	3.2	44
131	Effects of Electric Field Stress on a Î²-Amyloid Peptide. Journal of Physical Chemistry B, 2009, 113, 369-376.	2.6	83
132	Branched Substituents Generate Improved Supramolecular Ordering in Physisorbed Molecular Assemblies. Journal of Physical Chemistry C, 2009, 113, 4955-4959.	3.1	11
133	Polyareneâ€Functionalized Fullerenes in Carbon Nanotubes: Towards Controlled Geometry of Molecular Chains. Small, 2008, 4, 2262-2270.	10.0	21
134	Interactions of Aromatic Heterocycles with Water: The Driving Force from Freeâ€Jet Rotational Spectroscopy and Model Electrostatic Calculations. ChemPhysChem, 2008, 9, 1303-1308.	2.1	10
135	Shaping of a Conformationally Flexible Molecular Structure for Spectroscopy. Angewandte Chemie - International Edition, 2008, 47, 3174-3179.	13.8	29
136	Cadiotâ€“Chodkiewicz Active Template Synthesis of Rotaxanes and Switchable Molecular Shuttles with Weak Intercomponent Interactions. Angewandte Chemie - International Edition, 2008, 47, 4392-4396.	13.8	101
137	Double-wall carbon nanotubes: The outer shell may pattern the structure of the inner one. Chemical Physics Letters, 2008, 463, 139-140.	2.6	12
138	Growth of p- and n-Dopable Films from Electrochemically Generated C₆₀ Cations. Journal of the American Chemical Society, 2008, 130, 3788-3796.	13.7	35
139	The Erratic Emission of Pyrene on Gold Nanoparticles. ACS Nano, 2008, 2, 77-84.	14.6	60
140	Molecular Mechanism of Water Bridge Buildup: Field-Induced Formation of Nanoscale Menisci. Langmuir, 2008, 24, 6116-6120.	3.5	86
141	Singling out the Electrochemistry of Individual Single-Walled Carbon Nanotubes in Solution. Journal of the American Chemical Society, 2008, 130, 7393-7399.	13.7	99
142	Driving Force for the Adsorption of Sexithiophene on Gold. Journal of Physical Chemistry C, 2008, 112, 19516-19520.	3.1	11
143	Atomistic Simulation of â€œDrop-on-Demandâ€•Inkjet Dynamics. Journal of Physical Chemistry C, 2008, 112, 10616-10621.	3.1	5
144	On-the-Fly, Electric-Field-Driven, Coupled Electronâ^'Nuclear Dynamics. Journal of Physical Chemistry A, 2008, 112, 9650-9656.	2.5	36

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145	Self-assembly of semifluorinated n-alkanethiols on {111}-oriented Au investigated with scanning tunneling microscopy experiment and theory. Journal of Chemical Physics, 2007, 127, 024702.	3.0	11
146	Towards Understanding Different Spatial and Temporal Scales. AIP Conference Proceedings, 2007, , .	0.4	0
147	Extremely Strong and Readily Accessible AAAâˆ’DDD Triple Hydrogen Bond Complexes. Journal of the American Chemical Society, 2007, 129, 476-477.	13.7	103
148	Role of the Intracellular Cavity in Potassium Channel Conductivity. Journal of Physical Chemistry B, 2007, 111, 13993-14000.	2.6	13
149	Adsorption of Organic Molecules on Gold Electrodes. Journal of Physical Chemistry C, 2007, 111, 13879-13885.	3.1	22
150	Synthetic Molecular Motors and Mechanical Machines. Angewandte Chemie - International Edition, 2007, 46, 72-191.	13.8	2,428
151	Molecular Dynamics of Nanobubblesâ€™ Collapse in Ionic Solutions. ChemPhysChem, 2007, 8, 47-49.	2.1	13
152	Chargeâ€“Metal Interaction of a Carbon Nanotube. ChemPhysChem, 2007, 8, 1005-1008.	2.1	9
153	Dynamics of Thiolate Chains on a Gold Nanoparticle. Small, 2007, 3, 386-388.	10.0	42
154	C₆₀ on Gold: Adsorption, Motion, and Viscosity. Small, 2007, 3, 1694-1698.	10.0	19
155	An introduction to bubble dynamics. Physical Chemistry Chemical Physics, 2007, 9, 2447.	2.8	42
156	Potential energy surface and kinetics of the helixâ€“coil transition in a 33-peptide. Theoretical Chemistry Accounts, 2007, 118, 25-34.	1.4	3
157	Nonlinear optical properties of C60 with explicit time-dependent electron dynamics. Theoretical Chemistry Accounts, 2007, 118, 99-106.	1.4	9
158	Application of the Poisson-Nernst-Planck Theory with Space-Dependent Diffusion Coefficients to KcsA. Biophysical Journal, 2006, 91, 3162-3169.	0.5	39
159	Interactions in Single Wall Carbon Nanotubes/Pyrene/Porphyrin Nanohybrids. Journal of the American Chemical Society, 2006, 128, 11222-11231.	13.7	320
160	Surface Enhanced Second Harmonic Generation from Macrocycle, Catenane, and Rotaxane Thin Films:â€‰ Experiments and Theory. Journal of Physical Chemistry B, 2006, 110, 7648-7652.	2.6	9
161	Adsorption of Fumaramide [2]Rotaxane and Its Components on a Solid Substrate:â€‰ A Coverage-Dependent Study. Journal of Physical Chemistry B, 2006, 110, 17076-17081.	2.6	17
162	Clayâˆ’Fulleropyrrolidine Nanocomposites. Journal of the American Chemical Society, 2006, 128, 6154-6163.	13.7	46

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163	Self-organization of Rotaxane Thin Films into Spatially Correlated Nanostructures:Â Morphological and Structural Aspects. Journal of the American Chemical Society, 2006, 128, 526-532.	13.7	22
164	Ejection Dynamics of a Simple Liquid from Individual Carbon Nanotube Nozzles. Nano Letters, 2006, 6, 969-972.	9.1	11
165	Mono- and Bichromatic Electron Dynamics:Â LiH, a Test Case. Journal of Physical Chemistry A, 2006, 110, 5164-5172.	2.5	19
166	Molecular dynamics study of onset of water gelation around the collagen triple helix. Proteins: Structure, Function and Bioinformatics, 2006, 64, 711-718.	2.6	37
167	Mechanochemistry: targeted delivery of single molecules. Nature Nanotechnology, 2006, 1, 122-125.	31.5	95
168	Interactions in Concentric Carbon Nanotubes:â€‰ The Radius vs the Chirality Angle Contributions. Nano Letters, 2006, 6, 1950-1954.	9.1	19
169	Self-organization of nano-lines and dots triggered by a local mechanical stimulus. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 17650-17654.	7.1	26
170	Interaction Model for the Adsorption of Organic Molecules on the Silver Surface. Journal of Physical Chemistry B, 2006, 110, 5595-5601.	2.6	34
171	Simulation of some dynamical aspects of the photophysics of dye molecules encapsulated in a dendrimer. Journal of Luminescence, 2005, 111, 335-342.	3.1	8
172	Electric-field perturbations of ring currents in Ï€ systems. Chemical Physics Letters, 2005, 405, 136-141.	2.6	8
173	Intercage dynamics of C60 in doped crystals. Chemical Physics Letters, 2005, 405, 270-273.	2.6	1
174	Simple models for hydrophobic hydration. Chemical Society Reviews, 2005, 34, 1012.	38.1	39
175	Macroscopic transport by synthetic molecular machines. Nature Materials, 2005, 4, 704-710.	27.5	685
176	Patterning through Controlled Submolecular Motion: Rotaxane-Based Switches and Logic Gates that Function in Solution and Polymer Films. Angewandte Chemie - International Edition, 2005, 44, 3062-3067.	13.8	210
177	Continuous Chirality Measure in Reaction Pathways of Ruthenium-Catalyzed Transfer Hydrogenation of Ketones. Advanced Synthesis and Catalysis, 2005, 347, 792-802.	4.3	14
178	Ordering Fullerene Materials at Nanometer Dimensions. ChemInform, 2005, 36, no.	0.0	0
179	Charge-density oscillation on graphite induced by the interference of electron waves. Physical Review B, 2005, 71, .	3.2	85
180	Experimental and theoretical study of the adsorption of fumaramide [2]rotaxane on Au(111) and Ag(111) surfaces. Journal of Chemical Physics, 2005, 123, 244708.	3.0	21

#	Article	IF	Citations
181	The Collapse of Nanobubbles in Water. Journal of the American Chemical Society, 2005, 127, 8020-8021.	13.7	31
182	Guest Dynamics in Endohedrally Doped Fullerenes. Journal of Physical Chemistry B, 2005, 109, 15048-15051.	2.6	4
183	Asymmetric Indolylmaleimide Derivatives and Their Complexation with Zinc(II)â˜Cyclen. Journal of Physical Chemistry A, 2005, 109, 9443-9455.	2.5	21
184	Modeling the Stability and the Motion of DNA Nucleobases on the Gold Surface. Langmuir, 2005, 21, 2512-2518.	3.5	52
185	Favorable Entropy of Aromatic Clusters in Thermophilic Proteins. Journal of Physical Chemistry B, 2005, 109, 18184-18188.	2.6	5
186	Understanding the Cosolvation Effect of Dendrimers. Journal of Chemical Theory and Computation, 2005, 1, 194-200.	5.3	4
187	Intraresidue Distribution of Energy in Proteins. Journal of Physical Chemistry B, 2005, 109, 3586-3593.	2.6	1
188	Carbon Nanotubes in Electron Donorâ˜Acceptor Nanocomposites. Accounts of Chemical Research, 2005, 38, 871-878.	15.6	453
189	Unexpected Photophysical Properties of Symmetric Indolylmaleimide Derivatives. Journal of Physical Chemistry A, 2005, 109, 6440-6449.	2.5	31
190	Surface enhanced SHG from macrocycle, catenane and rotaxane thin films: experiments and theory. , 2005, 5724, 139.		1
191	Ordering Fullerene Materials at Nanometer Dimensions. Accounts of Chemical Research, 2005, 38, 38-43.	15.6	177
192	Motions In Catenanes And Rotaxanes. AIP Conference Proceedings, 2004, , .	0.4	0
193	Incorporation of Fullerene Derivatives into Smectite Clays:Â A New Family of Organicâ˜Inorganic Nanocomposites. Journal of the American Chemical Society, 2004, 126, 8561-8568.	13.7	47
194	The costly process of creating a cavity in n-octanol. Theoretical Chemistry Accounts, 2004, 112, 240.	1.4	9
195	Modelling of the Adsorption of C60 on the Au(110) Surface. ChemPhysChem, 2004, 5, 245-248.	2.1	33
196	Modulating Charge-Transfer Interactions in Topologically Different Porphyrinâ€"C60 Dyads.. ChemInform, 2004, 35, no.	0.0	0
197	The Mechanism of Formation of Amide-Based Interlocked Compounds: Prediction of a New Rotaxane-Forming Motif. Chemistry - A European Journal, 2004, 10, 4960-4969.	3.3	50
198	A Woodwardâ˜Hoffmann Approach to the C60Cluster Opening Leading to Homo[60]fullerenes. Journal of Physical Chemistry A, 2004, 108, 7135-7138.	2.5	9

#	Article	IF	Citations
199	Pyridinedicarboxamide Strands Form Double Helices via an Activated Slippage Mechanism. Journal of the American Chemical Society, 2004, 126, 2362-2367.	13.7	36
200	Electronic and mechanical coupling between guest and host in carbon peapods. Physical Review B, 2004, 69, .	3.2	52
201	Cyclic Voltammetry and Bulk Electronic Properties of Soluble Carbon Nanotubes. Journal of the American Chemical Society, 2004, 126, 1646-1647.	13.7	80
202	A Generic Basis for Some Simple Light-Operated Mechanical Molecular Machines. Journal of the American Chemical Society, 2004, 126, 12210-12211.	13.7	199
203	Title is missing!. Angewandte Chemie, 2003, 115, 2398-2402.	2.0	60
204	Modulating Charge-Transfer Interactions in Topologically Different Porphyrinâ€“C60 Dyads. Chemistry - A European Journal, 2003, 9, 4968-4979.	3.3	110
205	On the Cavitation Energy of Water. Chemistry - A European Journal, 2003, 9, 566-569.	3.3	18
206	Large Enhancement of the Nonlinear Optical Response of Reduced Fullerene Derivatives. Chemistry - A European Journal, 2003, 9, 1529-1534.	3.3	39
207	Remarkable Positional Discrimination in Bistable Light- and Heat-Switchable Hydrogen-Bonded Molecular Shuttles. Angewandte Chemie - International Edition, 2003, 42, 2296-2300.	13.8	187
208	Entropy-Driven Translational Isomerism: A Tristable Molecular Shuttle. Angewandte Chemie - International Edition, 2003, 42, 5886-5889.	13.8	103
209	Rotaxanesâ€“â€“novel photonic molecules. Optical Materials, 2003, 21, 39-44.	3.6	12
210	Unidirectional rotation in a mechanically interlocked molecular rotor. Nature, 2003, 424, 174-179.	27.8	862
211	The Free Energy of Nanobubbles in Organic Liquids. Journal of Physical Chemistry A, 2003, 107, 11253-11257.	2.5	10
212	Mechanical Interactions in All-Carbon Peapods. Journal of Physical Chemistry B, 2003, 107, 6986-6990.	2.6	37
213	Modeling the Adsorption of Alkanes on an Au(111) Surface. Langmuir, 2003, 19, 7335-7340.	3.5	57
214	Modulation of the Reduction Potentials of Fullerene Derivatives. Journal of the American Chemical Society, 2003, 125, 7139-7144.	13.7	66
215	Enantiomeric Excesses and Electronic Chirality Measure. Journal of the American Chemical Society, 2003, 125, 1975-1979.	13.7	23
216	Molecular Dynamics of a Dendrimerâ^'Dye Guestâ^'Host System. Journal of the American Chemical Society, 2003, 125, 7388-7393.	13.7	53

#	Article	IF	Citations
217	Kinetics of Place-Exchange Reactions of Thiols on Gold Nanoparticles. Langmuir, 2003, 19, 5172-5174.	3.5	119
218	Information Storage Using Supramolecular Surface Patterns. Science, 2003, 299, 531-531.	12.6	193
219	Photoisomerization of a rotaxane hydrogen bonding template: Light-induced acceleration of a large amplitude rotational motion. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 10-14.	7.1	185
220	C70Ph8 and C70Ph10: A computational and solid solution spectroscopic study. Journal of Chemical Physics, 2002, 116, 7621-7626.	3.0	19
221	Supramolecular self-assembled fullerene nanostructures. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 5075-5080.	7.1	191
222	Adsorption of a Benzylic Amide Macrocycle on a Solid Substrate:â€‰ XPS and HREELS Characterization of Thin Films Grown on Au(111). Journal of Physical Chemistry B, 2002, 106, 8739-8746.	2.6	40
223	From reactants to products via simple hydrogen-bonding networks: Information transmission in chemical reactions. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 4967-4971.	7.1	53
224	Organic Functionalized Carbon Nanotubes. AIP Conference Proceedings, 2002, , .	0.4	0
225	Permanent Chiral Twisting of Nonchiral Carbon Nanotubes. Journal of Physical Chemistry A, 2002, 106, 4795-4797.	2.5	13
226	Spontaneous Fabrication of Microscopic Arrays of Molecular Structures with Submicron Length Scales. Nano Letters, 2002, 2, 635-639.	9.1	21
227	The Effect of Mechanical Interlocking on Crystal Packing:â€‰ Predictions and Testing. Journal of the American Chemical Society, 2002, 124, 225-233.	13.7	83
228	Switching â€œOnâ€•and â€œOffâ€•the Expression of Chirality in Peptide Rotaxanes. Journal of the American Chemical Society, 2002, 124, 2939-2950.	13.7	118
229	Excited and ionic states of formamide: An excited-state photoelectron spectroscopy and ab initio study. Journal of Chemical Physics, 2002, 117, 8270-8280.	3.0	20
230	Structure and Photophysics of an Old, New Molecule:Â 1,3,6,8-Tetraazatricyclo[4.4.1.13,8]dodecane. Journal of the American Chemical Society, 2002, 124, 149-158.	13.7	10
231	Control of Supramolecular Shapes at Nanometer Level. AIP Conference Proceedings, 2002, , .	0.4	0
232	Understanding the properties of benzylic amide-based interlocked molecular architectures. AIP Conference Proceedings, 2002, , .	0.4	0
233	The Effect of Guest Inclusion on the Crystal Packing of p-tert-Butylcalix[4]arenes. Chemistry - A European Journal, 2002, 8, 4854-4866.	3.3	33
234	Solid-State Fingerprints of Molecular Threading Detected by Inelastic Neutron Scattering. ChemPhysChem, 2002, 3, 1038-1041.	2.1	7

#	Article	IF	Citations
235	Effect of potassium intercalation on the electronic and vibrational properties of benzylic amide [2]catenane films. Surface Science, 2002, 515, 45-52.	1.9	7
236	Dynamics of carbon clusters: chemical equilibration of rings and bi-cyclic rings. Chemical Physics Letters, 2002, 358, 359-367.	2.6	14
237	Isomers of C70Dimer. Journal of Physical Chemistry A, 2001, 105, 1140-1143.	2.5	10
238	Saturation versus inductive effects: the electrochemistry of the C70Ph2n (nâ€…=â€…1â€“5) series. Perkin Transactions II RSC, 2001, , 140-145.	1.1	16
239	Photoemission study of pristine and potassium intercalated benzylic amide catenane films. Surface Science, 2001, 474, 37-46.	1.9	22
240	Parallel (Face-to-Face) Versus Perpendicular (Edge-to-Face) Alignment of Electron Donors and Acceptors in Fullerene Porphyrin Dyads:Â The Importance of Orientation in Electron Transfer. Journal of the American Chemical Society, 2001, 123, 9166-9167.	13.7	157
241	Conformational Self-Recognition as the Origin of Dewetting in Bistable Molecular Surfaces. Journal of Physical Chemistry B, 2001, 105, 10826-10830.	2.6	57
242	Photophysical Properties of the Ground and Triplet State of Four Multiphenylated [70]Fullerene Compounds. ChemPhysChem, 2001, 2, 109-114.	2.1	13
243	A Quantum-Mechanical Description of Macrocyclic Ring Rotation in Benzylic Amide [2]Catenanes. Chemistry - A European Journal, 2001, 7, 1450-1454.	3.3	26
244	The inelastic neutron scattering of two benzylic amide [2]catenanes. Journal of Chemical Physics, 2001, 114, 5006-5011.	3.0	14
245	Evidence for ring spinning in rotaxanes induced with an alternate electric field. , 2000, 4106, 194.		1
246	Reducing Molecular Shuttling to a Single Dimension. Angewandte Chemie - International Edition, 2000, 39, 350-353.	13.8	74
247	Physical Consequences of a Mechanically Interlocked Architecture: Benzylic Amide Catenane NH Stretching Vibrations as Sensitive Probes for Weakly Hydrogen-Bonding Environments. ChemPhysChem, 2000, 1, 97-100.	2.1	19
248	Influencing intramolecular motion with an alternating electric field. Nature, 2000, 406, 608-611.	27.8	223
249	Nonlinear Optical Properties of Benzylic Amide [2] Catenanes: A Novel Versatile Photonic Material. Molecular Crystals and Liquid Crystals, 2000, 353, 545-559.	0.3	2
250	The Electrochemistry of C60Ph5Cl:â€‰ A Very Special Fullerene Derivative. Journal of the American Chemical Society, 2000, 122, 4209-4212.	13.7	23
251	Competition between Even and Odd Fullerenes:â€‰ C118, C119, and C120. Journal of Physical Chemistry A, 2000, 104, 9625-9629.	2.5	29
252	On the Distribution of Local Molecular Symmetry in Crystals. Journal of Physical Chemistry A, 2000, 104, 11439-11442.	2.5	9

#	Article	IF	Citations
253	13C NMR Patterns of Odd-Numbered C119 Fullerenes. Journal of Physical Chemistry A, 2000, 104, 3865-3868.	2.5	12
254	Physical Consequences of a Mechanically Interlocked Architecture: Benzylic Amide Catenane NH Stretching Vibrations as Sensitive Probes for Weakly Hydrogen-Bonding Environments. ChemPhysChem, 2000, 1, 97-100.	2.1	0
255	Scaling of the second hyperpolarisabilities of conjugated carbon systems: polyynes versus polyenes and fullerenes. Chemical Physics Letters, 1999, 313, 426-430.	2.6	16
256	C36, a hexavalent building block for fullerene compounds and solids. Chemical Physics Letters, 1999, 300, 369-378.	2.6	93
257	Third-Order Susceptibility of Li@C60. Advanced Materials, 1999, 11, 405-408.	21.0	27
258	Modeling Buckminsterfullerene Spinning in (C60)nClusters. Journal of the American Chemical Society, 1999, 121, 5281-5286.	13.7	18
259	Pentagon adjacency as a determinant of fullerene stability. Physical Chemistry Chemical Physics, 1999, 1, 2913-2918.	2.8	178
260	Carbon Rings Snapping. Journal of the American Chemical Society, 1999, 121, 10958-10961.	13.7	11
261	Simulation of STM Images from Commercially Available Software. Journal of the American Chemical Society, 1999, 121, 5392-5395.	13.7	20
262	Modeling the Spectroscopy of the Lowest Excited Singlet State of cis,trans-1,3,5,7-Octatetraene:â€‰ The Role of Symmetry Breaking and Vibronic Interactions. Journal of Physical Chemistry A, 1999, 103, 2220-2226.	2.5	15
263	Electrochemically Induced Dynamics of a Benzylic Amide [2]Catenane. Journal of Physical Chemistry B, 1999, 103, 10171-10179.	2.6	20
264	How Do Benzylic Amide [2]Catenane Rings Rotate?. Journal of the American Chemical Society, 1999, 121, 2364-2379.	13.7	69
265	C36:Â The Best Fullerene for Covalent Bonding. Journal of the American Chemical Society, 1999, 121, 3218-3219.	13.7	44
266	A Tight-Binding Treatment for13C NMR Spectra of Fullerenes. Journal of Physical Chemistry A, 1999, 103, 8738-8746.	2.5	55
267	Sum over orbitals scaling of the second hyperpolarisabilities of polyenic chains: a case study. Chemical Physics Letters, 1998, 285, 180-185.	2.6	6
268	Vibronic interactions in s-trans-butadiene. Chemical Physics Letters, 1998, 287, 275-281.	2.6	8
269	The hyperpolarisability of an endohedral fullerene: Li@C60. Chemical Physics Letters, 1998, 288, 131-137.	2.6	45
270	The large 1â€ˆ1Agâ€ˆâ€“â€œ2â€ˆ1Agâ€ˆCĩ…C and Câ€“C stretch vibronic interaction in all-trans polyenes. Chemical Physics Letters, 1998, 289, 118-124.	2.6	7

#	Article	IF	Citations
271	Experimental and theoretical studies of the low-lying electronic states of the simplest benzylic amide [2]catenane. Chemical Physics, 1998, 238, 421-428.	1.9	7
272	Growth and characterization of benzylic amide [2]catenane thin films. Thin Solid Films, 1998, 327-329, 321-325.	1.8	20
273	The vibrational spectroscopy of C60H36: An experimental and theoretical study. Chemical Physics, 1998, 232, 75-94.	1.9	50
274	High-Frequency Vibrations of the Simplest Benzylic Amide [2]Catenane. Journal of Physical Chemistry A, 1998, 102, 5782-5788.	2.5	19
275	Nuclear Motions of an Inclusion Complex of Calix[4]arene. Journal of Physical Chemistry A, 1998, 102, 6910-6915.	2.5	13
276	Controlling the Frequency of Macrocyclic Ring Rotation in Benzylic Amide [2]Catenanes. Journal of the American Chemical Society, 1998, 120, 6458-6467.	13.7	92
277	Structural Predictions for the C116Molecule. Journal of Physical Chemistry A, 1998, 102, 6835-6841.	2.5	27
278	Inelastic neutron scattering of large molecular systems: The case of the original benzylic amide [2]catenane. Journal of Chemical Physics, 1998, 109, 11094-11100.	3.0	18
279	Ab initio scaling of the second hyperpolarizabilities of carbon cages. Journal of Chemical Physics, 1997, 107, 5072-5075.	3.0	27
280	Stilbenoid molecules: An experimental and theoretical study of trans-1-(2-pyridyl)-2-(4-pyridyl)-ethylene and the parent molecule. Journal of Chemical Physics, 1997, 107, 1073-1078.	3.0	9
281	Energetics of C20and C22Fullerene and Near-Fullerene Carbon Cages. Journal of Physical Chemistry A, 1997, 101, 8339-8344.	2.5	40
282	Rotor-vibrator couplings in partially deuterated toluenes. Journal of Chemical Physics, 1997, 106, 6279-6287.	3.0	9
283	A Density Functional Study of the Vibrations of Three Oligomers of Thiophene. Journal of Physical Chemistry A, 1997, 101, 7283-7291.	2.5	33
284	Polarization Effects in Pushâ^'Pull Buckminsterfullerenes:Â A Semiempirical Study. Journal of Physical Chemistry A, 1997, 101, 3015-3020.	2.5	11
285	Energetics of Fullerenes with Octagonal Rings. Fullerenes, Nanotubes, and Carbon Nanostructures, 1997, 5, 747-768.	0.6	8
286	Semiempirical quantum-chemical assignment of the circular dichroism spectra of small chiral fullerenes. Chemical Physics, 1997, 223, 159-168.	1.9	19
287	Vibrational structure of C84 and Sc2@C84 analyzed by IR spectroscopy. Journal of Molecular Structure, 1997, 408-409, 359-362.	3.6	21
288	An Instanton approach to hindered torsions: methyl glycolate â€" a case study. Chemical Physics Letters, 1997, 271, 189-196.	2.6	8

#	Article	IF	Citations
289	Energetics of Fullerenes with Four-Membered Rings. The Journal of Physical Chemistry, 1996, 100, 6984-6991.	2.9	84
290	Propensity Rules for the Stability of Odd-Numbered Fullerenes:Â A Semiempirical Proposal. Journal of the American Chemical Society, 1996, 118, 2734-2739.	13.7	11
291	Evidence of Stringlike Behavior inall-trans-Octatetraene. Journal of the American Chemical Society, 1996, 118, 9178-9179.	13.7	7
292	Stability and IR spectra of isomers of C60F48. Journal of the Chemical Society Perkin Transactions II, 1996, , 155.	0.9	12
293	Energetics of fullerenes with heptagonal rings. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2203.	1.7	65
294	<title>New assignments in the 600-nm region of C<formula><inf><roman>60</roman></inf></formula></title>. , 1996, , .		0
295	The EEL epectrum of the triplet exciton of C60 and the theoretical analysis of its vibronic structure. Chemical Physics Letters, 1996, 250, 537-543.	2.6	19
296	Increasing cost of pentagon adjacency for larger fullerenes. Chemical Physics Letters, 1996, 250, 544-548.	2.6	130
297	Experimental and Theoretical Study of the Infrared, Raman, and Electronic Spectra of Two Isomers of C78ofC2vSymmetry. The Journal of Physical Chemistry, 1996, 100, 13399-13407.	2.9	45
298	C62:â€‰ Theoretical Evidence for a Nonclassical Fullerene with a Heptagonal Ring. The Journal of Physical Chemistry, 1996, 100, 15634-15636.	2.9	97
299	The intramolecular vibrations of prototypical polythiophenes. Journal of Chemical Physics, 1996, 104, 9704-9718.	3.0	44
300	The torsional spectrum of CH3CD3. Journal of Chemical Physics, 1996, 105, 8536-8542.	3.0	11
301	New Assignments in the 600 nm Region of C60:Â The Origins of the T1gand GgTransitions. The Journal of Physical Chemistry, 1996, 100, 10849-10853.	2.9	39
302	A generalized Stone - Wales map: energetics and isomerizations of carbon cages. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, 4895-4906.	1.5	14
303	The Raman activity of and : a computational semiempirical study. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, 5065-5075.	1.5	13
304	Validity of the essential states model in fullerenes. , 1995, , .		1
305	The Stone-Wales map for C60. Chemical Physics Letters, 1995, 235, 146-151.	2.6	49
306	Tunneling splittings from ab initio data: indoline, a test case. Chemical Physics Letters, 1995, 237, 279-285.	2.6	20

#	Article	IF	Citations
307	The S0-T1 transition of [1.1.1]propellane: a theoretical study. Chemical Physics Letters, 1995, 241, 445-449.	2.6	3
308	Charging and equilibration of fullerene isomers. Chemical Physics Letters, 1995, 243, 36-41.	2.6	65
309	Frequency-Dependent Second-Order Hyperpolarizability of Carbon Clusters: A Semiempirical Investigation. Journal of the American Chemical Society, 1995, 117, 6101-6108.	13.7	55
310	Dynamics of molecular inversion: An instanton approach. Journal of Chemical Physics, 1995, 102, 7024-7034.	3.0	40
311	Vibronic activity in trans,transâ€1,3,5,7 octatetraene: The S0â†'S1 spectrum. Journal of Chemical Physics, 1995, 103, 10492-10501.	3.0	29
312	Structural Motifs and the Stability of Fullerenes. The Journal of Physical Chemistry, 1995, 99, 8076-8081.	2.9	46
313	Electronic Absorption Spectra of Some Alkoxyl Radicals. An Experimental and Theoretical Study. Journal of the American Chemical Society, 1995, 117, 2711-2718.	13.7	74
314	Electrochemical Monitoring of Valence Bond Isomers Interconversion in Bipyridyl-C61 Anions. Journal of the American Chemical Society, 1995, 117, 6572-6580.	13.7	64
315	Franck-Condon Modeling of the Structure of the 1Ag-1Bu Electronic Transition of .alpha.,.omega. Diphenylpolyenes. Journal of the American Chemical Society, 1995, 117, 1621-1624.	13.7	9
316	Circumstellar carbon chain molecules: A density function theory study of CnO, n=3â€"9. Journal of Chemical Physics, 1995, 103, 6343-6349.	3.0	56
317	Energetics and isomerisation pathways of a lower fullerene. The Stoneâ€"Wales map for C40. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 1421-1423.	1.7	30
318	The resonance Raman spectrum of cyclobutene. Journal of Chemical Physics, 1995, 103, 5911-5918.	3.0	21
319	Triplet State Resonance Raman and Absorption Spectroscopy of a Configurationally Locked (Z)-Hexatriene: 1,2-Divinylcyclopentene. The Journal of Physical Chemistry, 1994, 98, 9437-9445.	2.9	10
320	Modeling of the Franck-Condon Structure of the Electronic Transitions of an Oligomer of Polydiacetylene. The Journal of Physical Chemistry, 1994, 98, 13157-13161.	2.9	18
321	Franckâ€"Condon modeling of the structure of the S0â†'S2 transition of trans, transâ€, cis, transâ€, and cis, cisâ€octatetraene. Journal of Chemical Physics, 1994, 101, 1842-1851.	3.0	29
322	Resonance Raman spectra and quantum chemical vibrational analysis of the C7H7â‹... and C7D7â‹... benzyl radicals. Journal of Chemical Physics, 1994, 100, 3503-3513.	3.0	25
323	The circular dichroism spectrum of C76. A quantum chemical study. Chemical Physics Letters, 1994, 224, 113-117.	2.6	22
324	Relative stabilities of C76 isomers. A numerical test of the fullerene isolated-pentagon rule. Chemical Physics Letters, 1994, 226, 219-225.	2.6	33

#	Article	IF	Citations
325	Preresonance Raman Spectrum of C76. The Journal of Physical Chemistry, 1994, 98, 7933-7935.	2.9	14
326	TheS0(1Ag)â€“S1(1B2u) vibronic transition in benzene: Anabinitiostudy. Journal of Chemical Physics, 1994, 100, 2458-2464.	3.0	60
327	Molecular Structure of Stilbene in the T1 State. Transient Resonance Raman Spectra of Stilbene Isotopomers and Quantum Chemical Calculations. The Journal of Physical Chemistry, 1994, 98, 2254-2265.	2.9	30
328	Resonance Raman activity in odd quanta of the trans bending vibration of acetylene: Strong vibronic coupling in the XÌƒ to Ãƒ and XÌƒ to BÌƒ transitions. Chemical Physics Letters, 1993, 205, 39-45.	2.6	4
329	Scattering of the vibrational frequencies of 13C12C60â¯. A Raman spectroscopy and quantum chemical study. Chemical Physics Letters, 1993, 211, 353-357.	2.6	10
330	The electronic structure and vibrational frequencies of the stable C76 isomer of D2 symmetry. Chemical Physics Letters, 1993, 208, 441-445.	2.6	42
331	Scaled ab initio force field of E- and Z-hexatriene in the S0 and T1 states. Chemical Physics, 1993, 178, 133-145.	1.9	10
332	Vibrational spectrum and harmonic force field of trimethylamine. The Journal of Physical Chemistry, 1993, 97, 581-595.	2.9	74
333	Theoretical study of the vibronic structure of the 1â€‰1A1â†'1â€‰1B2 and 1â€‰1A1â†'1â€‰3B2 electronic transitions in cyclopentadiene. Journal of Chemical Physics, 1993, 99, 3721-3729.	3.0	35
334	Assignment and vibrational analysis of the 600â€‚nm absorption band in the phenoxyl radical and some of its derivatives. Canadian Journal of Chemistry, 1993, 71, 1655-1662.	1.1	44
335	Light-induced oxygen incision of C60. Journal of the Chemical Society Chemical Communications, 1993, , 220.	2.0	67
336	Analysis of the Raman Spectra of A3C60 and A₆C₆₀. Molecular Crystals and Liquid Crystals, 1993, 234, 155-160.	0.3	4
337	Franckâ€“Condon structure of the S0â†'S1 and S0â†'S2 transitions in norbornadiene. Journal of Chemical Physics, 1993, 98, 14-20.	3.0	22
338	Inelastic neutron-scattering study of the intramolecular vibrations of the C70 fullerene. The Journal of Physical Chemistry, 1993, 97, 3641-3643.	2.9	38
339	Infrared fingerprints of nine fullerene C82 isomers: a semiempirical prediction. The Journal of Physical Chemistry, 1993, 97, 13575-13579.	2.9	41
340	The Franckâ€“Condon structure of the 1Aâ†'1B transition of cisâ€•and transâ€hexatriene: An ab initio modeling. Journal of Chemical Physics, 1993, 98, 4822-4829.	3.0	30
341	A study of the large amplitude motions of indoline through microwave spectroscopy andab initiocalculations. Molecular Physics, 1993, 78, 1561-1574.	1.7	18
342	Quantum Chemical Calculations of C60 Vibrational Frequencies and Electronic States. NATO ASI Series Series B: Physics, 1993, , 201-208.	0.2	0

#	Article	IF	Citations
343	Vibrational potentials of the low frequency outâ€ofâ€plane motion in the ground and excited singlet electronic states of 9,10â€dihydrophenanthrene. Journal of Chemical Physics, 1992, 96, 7229-7236.	3.0	11
344	Theoretical investigation of asymmetric methyl rotor dynamics in partially deuterated acetophenones. Journal of Chemical Physics, 1992, 96, 7973-7976.	3.0	8
345	Resonance Raman spectroscopy of the B1u region of benzene: Analysis in terms of pseudoâ€Jahnâ€“Teller distortion. Journal of Chemical Physics, 1992, 96, 2617-2628.	3.0	27
346	Interpretation of the vibrational structure of the emission and absorption spectra of C60. Journal of Chemical Physics, 1992, 97, 6496-6503.	3.0	165
347	Low-lying electronic excited states of Buckminsterfullerene anions. Journal of the American Chemical Society, 1992, 114, 2909-2913.	13.7	66
348	Microwave spectrum and ab initio calculations of indazole. Journal of Molecular Spectroscopy, 1992, 155, 1-10.	1.2	26
349	Local density functional theory calculation of the in-plane force field and vibrational frequencies of conjugated molecules: benzene and octatetraene. Chemical Physics, 1992, 164, 91-97.	1.9	12
350	The vibrational frequencies of C60. Chemical Physics Letters, 1992, 190, 174-178.	2.6	51
351	Prediction of the structure and the vibrational frequencies of a C84 isomer of D2 symmetry. Chemical Physics Letters, 1992, 189, 495-498.	2.6	24
352	The infrared and Raman active vibrational frequencies of C60 hexaanion. Chemical Physics Letters, 1992, 196, 303-310.	2.6	30
353	Theoretical analysis of spectra of short polyenes. Chemical Reviews, 1991, 91, 867-891.	47.7	309
354	QCFF/PI vibrational frequencies of some spherical carbon clusters. Journal of the American Chemical Society, 1991, 113, 6037-6040.	13.7	87
355	Observation and modeling of the recombination kinetics of diphenylmethyl radicals in the cavities of Na-X zeolite. The Journal of Physical Chemistry, 1991, 95, 10018-10024.	2.9	30
356	Annealing graphite-like structures. A Monte Carlo-quantum chemical study. Chemical Physics, 1991, 150, 39-45.	1.9	5
357	The T1 and T2 planar structures of butadiene. Chemical Physics Letters, 1991, 176, 7-10.	2.6	9
358	The infrared spectrum of a non conjugated conducting polymer. Chemical Physics Letters, 1991, 187, 642-648.	2.6	8
359	Automerization of s-cis butadiene. Chemical Physics Letters, 1991, 184, 191-194.	2.6	8
360	Franckâ€”Codon activity of totally symmetric modes in the absorption spectrum of cyclopentadiene. Chemical Physics Letters, 1991, 179, 131-136.	2.6	13

#	Article	IF	Citations
361	Inversion potentials in the ground and excited electronic states of 9,10â€dihydroanthracene as probed by the absorption and fluorescence spectra of jetâ€cooled molecules. Journal of Chemical Physics, 1991, 94, 3511-3516.	3.0	24
362	Ground- and excited-state conformational heterogeneity of the 2'-naphthylbutadiene chromophore of a fluorescent cholesterol analog probe. The Journal of Physical Chemistry, 1990, 94, 4439-4446.	2.9	8
363	New assignment of the vibrational structure of the V â†•N transition in ethylene-d4. Chemical Physics Letters, 1990, 174, 119-125.	2.6	26
364	Quantum chemical and vibronic analysis of the 1â€‰2B2â†”1â€‰2A2, 2â€‰2B2transition in benzylâ€h7and benzylâ€d7radicals. Journal of Chemical Physics, 1990, 93, 600-608.	3.0	41
365	Vibrational spectrum and harmonic force field of trimethylphosphine. The Journal of Physical Chemistry, 1990, 94, 4820-4831.	2.9	26
366	The missing fluorescence of sâ€trans butadiene. Journal of Chemical Physics, 1990, 93, 1235-1245.	3.0	64
367	Inversion of the dioxolanyl radical: an experimental and theoretical study. Journal of the American Chemical Society, 1990, 112, 4284-4290.	13.7	16
368	Theoretical analysis of the vibrational structure of the Tâ†N transition in ethylene. Journal of Chemical Physics, 1989, 91, 5926-5933.	3.0	20
369	Theoretical analysis of the force field of the lowest excited singlet state of trans-stilbene. The Journal of Physical Chemistry, 1989, 93, 5124-5128.	2.9	48
370	Quantum-chemical analysis of the propeller-shaped molecule [4,4,4]-propellahexaene. A study in heavy-atom tunneling. Chemical Physics, 1989, 130, 45-54.	1.9	15
371	Circumstellar carbon-chain molecules. Prediction of the infrared spectrum of SiC4. Chemical Physics Letters, 1989, 164, 517-519.	2.6	23
372	Absolute intensities of CH-stretching overtones in chloroform and deuterochloroform. Chemical Physics Letters, 1989, 154, 273-279.	2.6	40
373	On the 1Agâ†'1Bu absorption spectrum of four butadiene isotopomers. Chemical Physics Letters, 1989, 157, 515-520.	2.6	14
374	Comparison of synchronous and asynchronous hydrogen transfer mechanisms in free-base porphyrins. Chemical Physics, 1989, 136, 285-295.	1.9	35
375	Vibrationally modulated hyperfine coupling in the EPR spectrum of the oxiranyl radical. Chemical Physics, 1989, 139, 503-506.	1.9	4
376	Theoretical investigation of the inversion of the methylcyclopropyl radical. Journal of the American Chemical Society, 1989, 111, 2799-2802.	13.7	11
377	Theoretical study of the force field of the lowest singlet electronic states of long polyenes. Journal of Chemical Physics, 1989, 91, 6215-6224.	3.0	50
378	Franck-Condon activity of totally symmetric modes in trans- and cis-polyacetylenes. Chemical Physics Letters, 1988, 143, 153-162.	2.6	19

#	Article	IF	Citations
379	Quantum-chemical investigation of Franck-Condon and Jahn-Teller activity in the electronic spectra of Buckminsterfullerene. Chemical Physics Letters, 1988, 144, 31-37.	2.6	333
380	Theoretical study of the CC stretching vibrations in linked polyene chains: Nystatin. Chemical Physics Letters, 1988, 144, 437-444.	2.6	8
381	Quantum-chemical analysis of the absorption and emission spectra of coronene. Chemical Physics, 1988, 123, 175-185.	1.9	23
382	Why do the S0â†'S1(nï€*) and S0â†'T2(nï€*) transitions in acetophenone display different activity of the methyl group torsion?. Chemical Physics Letters, 1988, 153, 436-440.	2.6	2
383	Theoretical analysis of Franck-Condon and vibronic activity of the ag and b3g modes in the S0â†" S1 transitions in anthracene. Chemical Physics, 1988, 127, 17-29.	1.9	33
384	On the vibrational force fields of the ground state of trans- and cis-polyacetylenes. Chemical Physics Letters, 1988, 151, 526-530.	2.6	3
385	Inversion of the oxiranyl radical occurs by quantum-mechanical tunneling. Journal of the American Chemical Society, 1988, 110, 6721-6726.	13.7	22
386	Theoretical study of the force fields of the three lowest singlet electronic states of linear polyenes. Journal of Chemical Physics, 1988, 89, 3681-3688.	3.0	93
387	Vibronic coupling in polyenes and their derivatives. Interpretation of the absorption and emission spectra of a derivative of dodecahexaene. Journal of Chemical Physics, 1987, 87, 2505-2512.	3.0	41
388	Vibronic coupling in 1,2,4,5-tetrafluorobenzene: the double-minimum potential of the butterfly motion (Q11) in the state S1. The Journal of Physical Chemistry, 1987, 91, 4238-4240.	2.9	9
389	Correlation between the frequency of the Franck-Condon active Cî—»C ag stretch vibration and the excitation energy of the 1Bu electronic state in polyenes. Chemical Physics Letters, 1987, 141, 138-142.	2.6	26
390	Normal modes and ground state geometry of porphine. Evidence for dynamic instability of the D2h configuration. Chemical Physics Letters, 1987, 139, 401-406.	2.6	13
391	The effect of pressure on the electronic spectra of anthracene derivatives. Journal of Luminescence, 1987, 38, 311-313.	3.1	4
392	Quantum mechanical calculation of vibronic effects on the S2î—¸S0 transition of azulene. Chemical Physics, 1987, 113, 167-173.	1.9	14
393	Analysis of the vibronic structure of the 1A1g â†' 1B3g, 1B2u transition in biphenyl -h10 and -d10. Chemical Physics Letters, 1986, 129, 296-302.	2.6	6
394	Pseudoparity propensity rules for vibronic perturbations in neutral alternant hydrocarbons. Chemical Physics Letters, 1986, 131, 409-413.	2.6	18
395	Vibronically induced intensities by CNDO /S calculations: The Î½8/Î½6 intensity ratio in S1 al S0 transition in benzene. Chemical Physics, 1986, 108, 197-201.	1.9	6
396	Quantum-chemical analysis of vibrational intensity distributions in the S0-S1 absorption spectra and raman excitation profiles of azulene. Chemical Physics, 1986, 110, 421-430.	1.9	33

#	Article	IF	Citations
397	Vibronic coupling in polyenes: The frequency increase of the active Cî—»C ag stretching mode in the absorption spectra. Chemical Physics, 1986, 108, 187-195.	1.9	48
398	Vibronic coupling in the benzyl radical. Chemical Physics Letters, 1985, 115, 253-258.	2.6	43
399	Vibronic coupling between the lowest electronic states of biphenyl. Chemical Physics Letters, 1985, 120, 140-146.	2.6	23
400	Janus-Type Dendrimers Based on Highly Branched Fluorinated Chains with Tunable Self-Assembly and ¹⁹F Nuclear Magnetic Resonance Properties. Macromolecules, 0, , .	4.8	13